Journal of Molecular Structure, 268 (1992) 405
Elsevier Science Publishers B.V., Amsterdam

AUTHOR INDEX

Abdelaoui, O., 335
Akin, A.C., 67, 87
Almond, M.J., 51
Anderson, D.G., 143
Ang, H.-G., 389

Barron, D.A., 143
Bohn, R.K., 97, 107, 123
Brzezinski, B., 61

Carlsen, P.H.J., 263
Cradock, S., 143

Dakkouri, M., 135
Domalewski, W., 311
Dunne, S.J., 373
Durig, J.R., 143

Edwards, H.G.M., 13, 353, 363

Farag, M.S., 107, 123
Fawcett, V., 353

Giorgini, M.G., 23
Gribov, L.A., 191, 223, 237
Grosser, M., 135

Harmon, K.M., 67, 77, 87
Herrebout, W.A., 293

Iijima, K., 315

Jhon, M.S., 169
Johnson, A.F., 363

Klimovitskii, E.N., 321
Knowles, A., 13
Koča, J., 263
Kon, M., 155
Konaka, S., 155
Kooijman, H., 283
Kroon, J., 283
Kurokawa, H., 155
Kwik, W.-L., 389

Lewis, I.R., 363
Liedle, S., 389
Liefooghe, H.H., 293
López-Navarette, J.T., 249
Lunelli, B., 23
Lee, Y.W., 389

Mack, H.G., 135
Maitland, D.J., 363
Mandai, Y., 41
Marciniak, B., 61
Mastryukov, V.S., 307, 395
Matsuura, H., 41
Mlochowski, J., 311
Mutarelli, S.R., 347

Negri, F., 23
Nikitin, O.Y., 223, 237
Novosadov, B.K., 223, 237

Oberhammer, H., 135, 389
Ohno, K., 41
Onuma, S., 315
Orlandi, G., 23
Ott, C.M., 107, 123

Pappalardo, L.M., 77
Paszyc, S., 61

Quirante, J.J., 249

Radhakrishnan, J., 107
Ramírez, F.J., 249
Rankin, D.W.H., 143
Rao, C.N.R., 1
Rice, D.A., 51
Rose, S.J., 353

Samdal, S., 395
Santos, P.S., 347
Schapin, I.Y., 307
Schilf, W., 311
Schriver, A., 335
Schriver, L., 335
Shagidullin, R.R., 321
Shakirov, I.Kh., 321
Shin, J.K., 169
Smith, D.N., 353
Snider, B.L., 77
Sobolev, P.N., 321
Sorenson, S.A., 97, 107, 123
Stefaniak, L., 311
Strel'nik, D.Yu., 321
Sullivan, J.F., 143
Summers, L.A., 373
Syper, L., 311

Takeuchi, H., 155
Tanaka, Y., 315
True, N.S., 97, 107, 123

van der Veken, B.J., 293
van Eijck, B.P., 283
Varma, V., 1
Varnali, T., 181
von Nagy-Felsobuki, E., 373

Webb, G.A., 311
Webb, N., 363

Yang, J.H., 169
Yates, C.A., 51

Zinovyev, K.A., 191
Zundel, G., 61

Journal of Molecular Structure, 268 (1992) 406–408
Elsevier Science Publishers B.V., Amsterdam

SUBJECT INDEX

A_3H_8,
Inverse "bond length/bond angle" relationship. Part 4. Ab initio study of A_3H_8 (A = C, Si, Ge), 395
Alanine dipeptide,
The structural variation and probability redistribution in alanine dipeptide conformers by hydration, 169
Anisaldehyde,
Rotational spectra of *p*-anisaldehyde. Assignment of the planar conformers and observation of torsionally excited states, 107
Temperature-dependent low-resolution microwave studies of *m*-iodoanisole, *m*-bromoanisole, *m*-nitroanisole and *m*-anisaldehyde, 123

Bis(trifluoromethyl)arsinous azide,
Gas-phase structure of bis(trifluoromethyl)arsinous azide $(CF_3)_2AsN_3$, 389
Bond angle,
Inverse "bond length/bond angle" relationship: C–H versus H–C–H, 307
Bond length,
Inverse "bond length/bond angle" relationship: C–H versus H–C–H, 307
m-Bromoanisole,
Temperature-dependent low-resolution microwave studies of *m*-iodoanisole, *m*-bromoanisole, *m*-nitroanisole and *m*-anisaldehyde, 123

$CBrCl_3$,
Matrix reaction of the oxygen atom with the $CBrCl_3$ molecule. Identification of phosgene complexes with Cl_2 and Br_2, 335
CH_3/CF_3 substitution,
On the CH_3/CF_3 substitution effect. The gas-phase structure of 1,1,1,3,3,3-hexafluoropropane, 135
Chlorotetrafluorosilicate(IV) ion,
The preparation and Raman spectroscopic study of the chlorotetrafluorosilicate(IV) ion, SiF_4Cl^-, 353
Complex molecules,
Engineering calculations of IR spectra of complex molecules, 191
Crystal structures,
Molecular dynamics simulations of crystal structures containing charged molecules, 283

2,2-Dialkyl-1,3-dithio-5,6-benzo-cycloheptenes,
Raman spectra and conformations of 2,2-dialkyl-1,3-dithio-5,6-benzocycloheptenes: coexistence of chair, boat and twist-boat forms, 321
Diethyl cadmium,
A vibrational spectroscopic study of diethyl cadmium in gas, liquid, solid and matrix-isolated states, 51
Dimethylpiperazine dioxide,
Hydrogen bonding. Part 41. Stoichiometry, thermodynamics of dissociation, and IR spectra of the hydrates of *N*,*N*-dimethylpiperazine dioxide, 67
Dimethyl(methylthio)phosphine,
Conformational stability and molecular structure of dimethyl(methylthio)-phosphine from electron diffraction studies and ab initio calculations, 143

Glycine,
Harmonic force field for the glycine molecule by semiempirical methods, 249
Gossypol,
The tautomerization of gossypol as a function of the presence of Ni^{2+}, Cu^{2+} or Zn^{2+} cations, 61

Hexafluoroacetylacetone,
Internal rotation of trifluoromethyl groups in hexafluoroacetylacetone, 315
Hexafluoropropane,
On the CH_3/CF_3 substitution effect. The gas-phase structure of 1,1,1,3,3,3-hexafluoropropane, 135
Hydrazonium sulfate,

An infrared and Raman study of the phase transitions and the torsional barrier in hydrazonium sulfate, $N_2H_6SO_4$, 1

Hydrogen bonding,
Hydrogen bonding. Part 41. Stoichiometry, thermodynamics of dissociation, and IR spectra of the hydrates of *N,N*-dimethylpiperazine dioxide, 67
Hydrogen bonding. Part 42. Proposed mechanism for the dissolution of succinic acid by fluoride ion, 77
Hydrogen Bonding. Part 43. IR and thermodynamic study of the stochiometry and stability of hydrates of triethylenediamine oxide, 87

Insect pheromones,
Conformational behavior of insect pheromones and analogues. Part II, 263

m-Iodoanisole,
Temperature-dependent low-resolution microwave studies of *m*-iodoanisole, *m*-bromoanisole, *m*-nitroanisole and *m*-anisaldehyde, 123

p-Isopropylbenzaldehyde,
Rotational spectra of *p*-isopropylbenzaldehyde: assignment of two conformers and observation of torsionally excited states, 97

Jahn–Teller mode enhancement,
Resonance Raman effect of the tetrathiosquarate ion: another example of Jahn-Teller mode enhancement, 347

Large molecular systems,
A general approach for calculating the electronic states of large molecular systems, 223
An approximate method of computing electronic characteristics of large molecular systems in the ground electronic state, 237

Matrix-isolated states,
A vibrational spectroscopic study of diethyl cadmium in gas, liquid, solid and matrix-isolated states, 51

Methanol,
The orientation of the dipole change for the OH stretch in methanol and nitric acid, 293

Methyl isonicotinate,
Conformational studies by liquid crystal NMR and ab initio calculations: methyl nicotinate and methyl isonicotinate, 155

Methyl nicotinate,
Conformational studies by liquid crystal NMR and ab initio calculations: methyl nicotinate and methyl isonicotinate, 155

Molecular conformation,
Vibrational spectra and molecular conformation of taurine and its related compounds, 41

Nickel(II) formate,
Vibrational spectroscopic study of nickel(II) formate, $Ni(HCO_2)_2$, and its aqueous solution, 13

Nitric acid,
The orientation of the dipole change for the OH stretch in methanol and nitric acid, 293

m-Nitroanisole,
Temperature-dependent low-resolution microwave studies of *m*-iodoanisole, *m*-bromoanisole, *m*-nitroanisole and *m*-anisaldehyde, 123

OH stretch,
The orientation of the dipole change for the OH stretch in methanol and nitric acid, 293

Organoselenium compounds,
A ^{1}H, ^{13}C, ^{15}N and ^{77}Se NMR study of three organoselenium compounds, 311

Phosgene complexes,
Matrix reaction of the oxygen atom with the $CBrCl_3$ molecule. Identification of phosgene complexes with Cl_2 and Br_2, 335

Polybutadiene,
Vibrational and NMR spectroscopic studies of a thiolsulphonate produced from the non-catalytic hydrogenation of polybutadiene, 363

Squaric acid,
Vibrational analysis of 1,2-dihydroxycyclobuten-3,4-dione (squaric acid) as a nearly-free molecule, 23

Succinic acid,
Hydrogen bonding. Part 42. Proposed mechanism for the dissolution of succinic acid by fluoride ion, 77

Taurine,
Vibrational spectra and molecular conformation of taurine and its related compounds, 41
Tautomerization,
The tautomerization of gossypol as a function of the presence of Ni^{2+}, Cu^{2+} or Zn^{2+} cations, 61
Tetrathiosquarate ion,
Resonance Raman effect of the tetrathiosquarate ion: another example of Jahn-Teller mode enhancement, 347
Thiobispyridines,
The photoelectron spectra of thiobispyridines, 373
Thiolsulphonate,
Vibrational and NMR spectroscopic studies of a thiolsulphonate produced from the non-catalytic hydrogenation of polybutadiene, 363
Torsionally excited states,
Rotational spectra of *p*-anisaldehyde. Assignment of the planar conformers and observation of torsionally excited states 107
Rotational spectra of *p*-isopropylbenzaldehyde: assignment of two conformers and observation of torsionally excited states, 97
Triethylenediamine oxide,
Hydrogen bonding. Part 43. IR and thermodynamic study of the stoichiometry and stability of hydrates of triethylenediamine oxide, 87
Trifluoromethyl groups,
Internal rotation of trifluoromethyl groups in hexafluoroacetylacetone, 315
1,1,2-Trisubstituted cyclohexanes,
Molecular mechanics application to 1,1,2-trisubstituted cyclohexanes, 181